



PERGAMON

Journal of Quantitative Spectroscopy &
Radiative Transfer 63 (1999) 231–236

Journal of
Quantitative
Spectroscopy &
Radiative
Transfer

www.elsevier.com/locate/jqsrt

Brief communication

Single-expansion EBCM computations for osculating spheres

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Abstract

We show that the standard, single-expansion extended boundary condition method provides convergent scattering results for osculating dielectric spheres and discuss the implications of this result. Published by Elsevier Science Ltd.

1. Introduction

The extended boundary condition method (EBCM), otherwise known as the single-expansion version of the *T*-matrix method, is an exact technique for computing electromagnetic scattering by small particles based on numerically solving Maxwell's equations [1,2]. Although in principle this technique can be applied to arbitrarily shaped particles, most practical applications of EBCM have dealt with rotationally symmetric particles such as spheroids, finite circular cylinders, and so-called Chebyshev particles [2]. In this Brief Communication we apply EBCM to a new class of particles, namely, osculating spheres. This research is motivated not only by the natural desire to expand the range of shapes treated with EBCM, but also by the fact that the application of the multi-expansion superposition *T*-matrix method (STM) to osculating spheres seems to produce divergent results [3,4].

2. Computations

Unlike STM [5], EBCM uses a single expansion of the incident, internal, and scattered fields in vector spherical wave functions. Computations for osculating spheres (i.e., spheres with the

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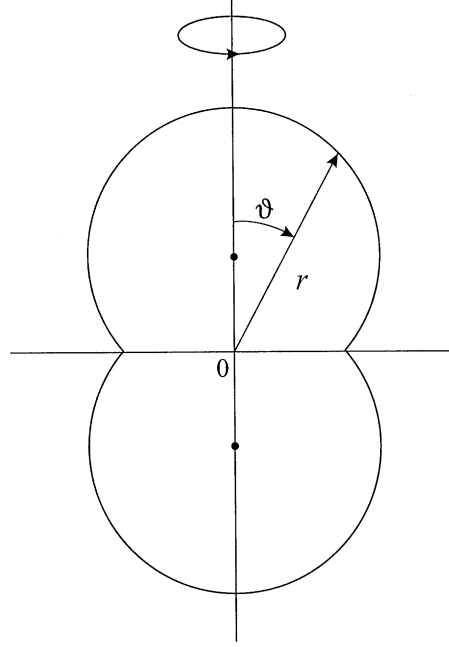


Fig. 1. Spherical coordinates used to specify the shape of an osculating sphere with equal components.

distance between their centers smaller than the sum of their radii; see Fig. 1) required a rather straightforward modification of the single-expansion T -matrix code described in [6] and available at <http://www.giss.nasa.gov/~crmim>. Specifically, we have added a simple subroutine which computes the shape of the particle, $r(\vartheta, \varphi)$, and the partial derivative $\partial r(\vartheta, \varphi)/\partial \vartheta$. The shape of a particle formed by a pair of identical osculating spheres in the spherical coordinate system with the z -axis directed along the line connecting the centers of the spheres (Fig. 1) is given by the following simple expression:

$$r(\vartheta, \varphi) = \begin{cases} R(f \cos \vartheta + \sqrt{1 - f^2 \sin^2 \vartheta}), & \vartheta < \pi/2, \\ R(-f \cos \vartheta + \sqrt{1 - f^2 \sin^2 \vartheta}), & \vartheta > \pi/2, \end{cases} \quad (1)$$

where R is the radius of the component spheres, $f = d/(2R)$, and d is the distance between the sphere centers. Furthermore,

$$\frac{\partial r(\vartheta, \varphi)}{\partial \vartheta} = \begin{cases} -Rf \sin \vartheta \left[1 + \frac{f \cos \vartheta}{\sqrt{1 - f^2 \sin^2 \vartheta}} \right], & \vartheta < \pi/2, \\ Rf \sin \vartheta \left[1 - \frac{f \cos \vartheta}{\sqrt{1 - f^2 \sin^2 \vartheta}} \right], & \vartheta > \pi/2. \end{cases} \quad (2)$$

The T -matrix code computes the optical-cross sections, the asymmetry parameter of the phase function, and the elements of the scattering matrix for randomly oriented particles. Since osculating spheres are particles with a plane of symmetry, the scattering matrix has a simple block-diagonal

Table 1
Extinction cross section and asymmetry parameter of the phase function for randomly oriented osculating spheres with $f = 1$ (bisphere with touching components), 0.5, 0.2, and 0 (single sphere)

f	$C_{\text{ext}} (\mu\text{m}^2)$	g
1	4.861	0.8573
0.5	4.185	0.8617
0.2	3.360	0.8615
0	2.654	0.8550

structure,

$$F(\Theta) = \begin{bmatrix} a_1(\Theta) & b_1(\Theta) & 0 & 0 \\ b_1(\Theta) & a_2(\Theta) & 0 & 0 \\ 0 & 0 & a_3(\Theta) & b_2(\Theta) \\ 0 & 0 & -b_2(\Theta) & a_4(\Theta) \end{bmatrix}, \quad (3)$$

where Θ is the scattering angle, and has only six independent elements [7]. The (1,1)-element of the scattering matrix (i.e., the phase function) satisfies the standard normalization condition,

$$\frac{1}{2} \int_0^\pi a_1(\Theta) \sin \Theta \, d\Theta = 1. \quad (4)$$

We have found that although the accuracy of single-expansion T -matrix computations for osculating spheres depends on the particle refractive index m and size parameter $x = 2\pi R/\lambda$ (λ is wavelength) as well as on f , convergent results can be obtained for a rather wide range of these parameters. As an example, Fig. 1 and Table 1 show results computed with an extended-precision FORTRAN code for $m = 1.31$, $R = 0.5 \mu\text{m}$, $\lambda = 0.6283 \mu\text{m}$, and $f = 0$ (single sphere), 0.2, and 0.5. For comparison, we also show results for a bisphere with touching components ($f = 1$) obtained with the superposition T -matrix code described in [8]. In all cases the size of the T matrix was increased in unit steps until the extinction and scattering cross-sections converged within 0.01%. The physical correctness of the results was checked using the general relationships derived in [9,10]. Furthermore, we have made sure that EBCM results for $f = 0$ (single sphere) exactly reproduce the corresponding Lorenz–Mie results.

Not surprisingly, the single-sphere curves in Fig. 1 exhibit the largest amplitude of oscillations caused by interference effects, whereas the amplitude of oscillations for other particles is reduced by averaging over orientations. The growth of the average projected area with increasing f causes a notable increase of the extinction cross section (Table 1) and the forward-scattering phase function value, $a_1(0^\circ)$. Although for spheres $a_2(\Theta) \equiv a_1(\Theta)$ and $a_4(\Theta) \equiv a_3(\Theta)$, the results for nonspherical particles with $f > 0$ in Fig. 1 show significant differences between these scattering matrix elements.

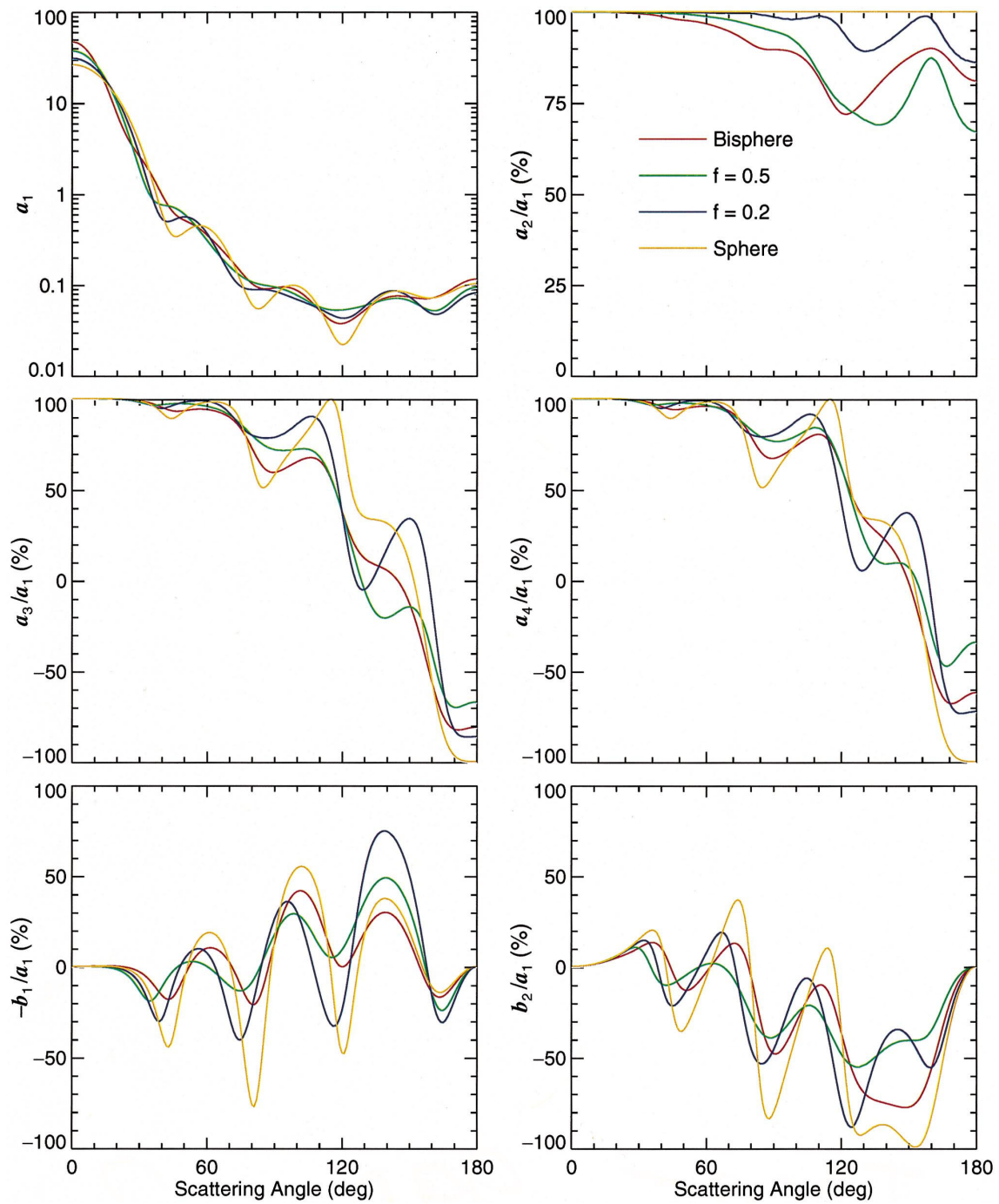


Fig. 2. Elements of the scattering matrix versus scattering angle for randomly oriented osculating spheres with $f = 1$ (bisphere with touching components), 0.5, 0.2, and 0 (single sphere).

Note that even with the extended-precision code, we could not obtain convergence for $f > 0.5$ for the same m , R , and λ . Apparently, this can be explained by the sensitivity of single-expansion EBCM computations to increasing concavity of the particle shape noted earlier by Mugnai and Wiscombe [11] in their calculations for Chebyshev particles.

3. Discussion and conclusions

Our results demonstrate that EBCM can be successfully applied to osculating spheres. On the other hand, the results of [3,4] suggest that the multi-expansion STM, while providing convergent results for bispheres with separated or touching components ($f \geq 1$) [8], produces divergent results for osculating spheres ($f < 1$). Furthermore, the performance of EBCM improves with decreasing f , in contrast to the behavior of STM. It is important to realize that STM for bispheres with touching or separated components does not rely on the so-called Rayleigh hypothesis (RH), but becomes dependent on RH for $f < 1$. (RH states that the expansion of the scattered field in outgoing spherical functions is valid in the region between the particle surface and its smallest circumscribing sphere.) Similar convergence problems are encountered with the point-matching technique, which also explicitly relies on RH [12]. On the other hand, the derivation of EBCM in [13] completely avoids the use of RH. Therefore, it seems logical to suggest that the success of EBCM in computations for osculating spheres may be explained by EBCM not relying on RH.

This result may be important since it has been shown that EBCM can be derived from RH [14,15]. The title and conclusions of [14] may seem to suggest that EBCM is equivalent to the method of RH. However, the fact that EBCM can be derived from RH only means that RH is a sufficient condition of validity of EBCM, but not the necessary condition. Therefore, one should not exclude the possibility that EBCM may be valid even when RH is violated [16].

Acknowledgements

We thank David Brown and Cornelis V.M. van der Mee for careful reading of the manuscript and valuable comments. This research was sponsored by the NASA Radiation Science Program managed by Robert Curran.

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